

DISCOVERY OF DATIVE BONDING OF BERYLLIUM FLUORIDE ANION BY PHOTOELECTRON VELOCITY MAP IMAGING SPECTROSCOPY

MALLORY THEIS, *Department of Chemistry, Emory University, Atlanta, GA, USA*; PEARL JEAN, *Chemistry Department, Emory University, Atlanta, Georgia, United States*; MICHAEL HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA, USA*.

Beryllium can exhibit unusually strong attractive interactions under conditions where it is nominally a closed-shell atom. Two prominent examples are the Be₂ dimer and the He-BeO complex. Most recently, we examined the bonding of a similarly interesting molecule, the closed-shell Be-F⁻ anion. This molecule preserves the closed-shell character of the atoms as the electron affinity of F is high (328.16 kJ mol⁻¹) while that of Be is negative. Photoelectron velocity map imaging spectroscopy, in conjunction with coupled cluster electronic structure calculations, were used to determine the vibrational frequency for BeF⁻ and the electron affinity of BeF (approximately 8700 cm⁻¹). The latter has been used to determine a lower bound of 28480 cm⁻¹ (343 kJ mol⁻¹) for the bond energy of BeF⁻. The electronic structure calculations yielded predictions that were in good agreement with the observed data. A natural bond orbital analysis shows that BeF⁻ is primarily bound by a dative interaction.